Description of .cif file of Hydroxy Apatite

1) _chemical_formula_sum -----> 'Ca$_5$HO$_{13}$P$_3$'

The sum formula for the content of the unit cell or asymmetric unit.

2) _chemical_name_mineral -----> Apatite-(CaOH)

Mineral name. Here "Apatite-(CaOH)" indicates hydroxy-apatite with Ca and OH.

3) _space_group_IT_number ----------> 176
_symmetry_space_group_name_Hall ----> '-P 6c'
_symmetry_space_group_name_H-M ----> 'P 63/m'

IT number 176 = International Tables space group 176.

Hall symbol (explicit symmetry operations): -P 6c.

Hermann–Mauguin (H–M) symbol: P 63/m.

This describes the symmetry properties of the crystal lattice(here a hexagonal space group).

4) _cell_angle_alpha ---------->90
_cell_angle_beta ---------->90
_cell_angle_gamma -----> 120

The angles between lattice vectors (for hexagonal systems):

$\alpha = \beta = 90°, \gamma = 120°$

5) _cell_length_a --------> 9.424
_cell_length_b --------> 9.424
_cell_length_c --------> 6.879

Lattice constants (in Å): a = b (hexagonal lattice),c different

6) _cell_volume 529.086

Unit cell volume in Å^3.

7) _cell_formula_units_Z 2

Number of formula units per unit cell.

8) _exptl_crystal_density_diffrn 3.153

Density computed from diffraction data (g/cm³).

9)

*loop_*

_symmetry_equiv_pos_as_xyz

x,y,z

-x+y,-x,1/2-z

x-y,x,1/2+z

y,-x+y,-z

-y,x-y,z

x,y,1/2-z

-x,-y,1/2+z

x-y,x,-z

-x+y,-x,z

-y,x-y,1/2-z

y,-x+y,1/2+z

-x,-y,-z

- **loop_** : begins a table of space-group symmetry operations.
- **_symmetry_equiv_pos_as_xyz:** lists each symmetry operation in algebraic x,y,z notation (the positions mapping).
- Each line is an operator that maps coordinates of one asymmetric unit atom to equivalent positions in the cell.
- The number of lines equals the number of symmetry operations in the given space group (here 12 operations are listed).

- R_0 : (x, y) −rotation 0°(identity in plane)
- R_{60}: $(-y, x+y)$— rotation $+60°$
- R_{120}: $(-x+y, -x)$— rotation $+120°$
- R_{180}: $(-x, -y)$— rotation $180°$
- R_{240}: $(y, -x+y)$— rotation $+240°$
- R_{300}: $(x-y, x)$--rotation $+300°$

a) x,y,z

Mapping:

$$(x', y', z') = (x, y, z)$$

How to use: take a point $(x, y, z)$and it stays the same.
Planar operation: R_0(identity, 0°).
Z behavior: unchanged.
Symmetry element name: Identity. (No change — the reference operation.)

b) -x+y,-x,1/2-z

Mapping:

$$(x', y', z') = (-x+y, -x, \frac{1}{2}-z)$$

How to apply: replace x by $-x+y$, y by $-x$, and z by $\frac{1}{2}-z$.
Planar operation: matches R_{120}(rotation by $+120°$in the basal plane).
Z behavior: $z \mapsto \frac{1}{2}-z$. This is a combination of a reflection/inversion of the z-coordinate (turning z into $-z$) plus a half-cell translation along c(the $\frac{1}{2}$).
Symmetry element name / interpretation: 120° rotation

combined with a mirror/inversion in the plane + a $c/2$ translation — physically this is the effect of the 6_3 screw/mirror content of $P6_3/m$. When applied to an atom at z, it sends it to the reflected position across a horizontal mirror and moves it by $+\frac{1}{2}$in c-direction.

c) x-y,x,1/2+z

Mapping:

$$(x', y', z') = (x - y,\ x,\ \frac{1}{2} + z)$$

How to apply: set $x' = x - y, y' = x, z' = z + \frac{1}{2}$.

Planar operation: R_{300}(rotation by $+300°$or $-60°$).

Z behavior: $z \mapsto z + \frac{1}{2}$ a pure translation by half a unit along c(no sign inversion of z).

Symmetry element name / interpretation: $+300°$**rotation with a half-cell translation along** c— this is characteristic of a component of the 6_3 screw (rotation + $c/2$).

d) y,-x+y,-z

Mapping:

$$(x', y', z') = (y,\ -x + y,\ -z)$$

How to apply: rotate in-plane as $R_{240}$and invert z.

Planar operation: R_{240}(rotation by $+240°$).

Z behavior: $z \mapsto -z$(pure inversion of the z coordinate, i.e. reflection through the plane $z = 0$ or inversion through center depending on context).

Symmetry element name / interpretation: 240° rotation + reflection (or inversion) perpendicular to c— it flips the sign of z.

e) -y,x-y,z

Mapping:

$$(x', y', z') = (-y,\ x - y,\ z)$$

How to apply: planar transform $(-y,\ x-y)$, $z$unchanged.
Planar operation: this expression is algebraically equivalent (modulo hexagonal lattice translations) to R_{60}(rotation by $+60°$); different but equivalent forms appear because of the hexagonal lattice basis. Concretely this is one of the $60°$-family maps.
Z behavior: $z$unchanged.
Symmetry element name / interpretation: +60° rotation (pure in-plane rotation) — no translation along c.

f) x,y,1/2-z
Mapping:

$$(x', y', z') = (x,\ y,\ \frac{1}{2} - z)$$

How to apply: keep x, ysame; send $z$to $\frac{1}{2} - z$.
Planar operation: identity in plane (R_0).
Z behavior: reflection/inversion of $z$combined with a $c/2$translation.
Symmetry element name / interpretation: horizontal mirror combined with a $c/2$shift (this is the mirror/inversion-related part of the space group acting at the origin).

g) -x,-y,1/2+z
Mapping:

$$(x', y', z') = (-x,\ -y,\ \frac{1}{2} + z)$$

How to apply: invert both in-plane fractional coordinates (180° rotation) and translate $z$by $+\frac{1}{2}$.
Planar operation: R_{180}(180° rotation).
Z behavior: $z \mapsto z + \frac{1}{2}$(pure half-cell translation along c).
Symmetry element name / interpretation: 180° rotation + $c/2$translation.

h) x-y,x,-z

Mapping:

$$(x', y', z') = (x - y,\ x,\ -z)$$

How to apply: planar $R_{300}(x - y, x)$ and invert z.
Planar operation: R_{300}(rotation by $+300°$).
Z behavior: $z \mapsto -z$.
Symmetry element name / interpretation: 300° rotation + reflection/inversion across plane perpendicular to c.

i) -x+y,-x,z

Mapping:

$$(x', y', z') = (-x + y,\ -x,\ z)$$

How to apply: planar $R_{120}$and leave $z$unchanged.
Planar operation: R_{120}(rotation by $+120°$).
Z behavior: unchanged.
Symmetry element name / interpretation: 120° rotation (pure in-plane rotation).

j) -y,x-y,1/2-z

Mapping:

$$(x', y', z') = (-y,\ x - y,\ \frac{1}{2} - z)$$

How to apply: planar map equivalent to R_{60}(or its equivalent lattice-congruence form) and $z \mapsto \frac{1}{2} - z$.
Planar operation: +60° rotation family (same family as line 5)
Z behavior: reflect/invert $z$and translate by $+\frac{1}{2}$.
Symmetry element name / interpretation: 60° rotation combined with mirror/inversion and a $c/2$**translation** (another 6_3/m-type operation).

k) y,-x+y,1/2+z

Mapping:

$$(x', y', z') = (y,\ -x + y,\ \frac{1}{2} + z)$$

How to apply: planar $R_{240}$and shift $z$by $+\frac{1}{2}$.
Planar operation: R_{240}(rotation by $+240°$).
Z behavior: $z \mapsto z + \frac{1}{2}$.
Symmetry element name / interpretation: 240° rotation + $c/2$translation.

l) **-x,-y,-z**
Mapping:

$$(x', y', z') = (-x, \ -y, \ -z)$$

How to apply: invert all three fractional coordinates (center of symmetry/inversion through origin).
Planar operation: $R_{180}$for the in-plane part, but because $z$is also inverted this is a **true inversion** (centrosymmetric operation).
Z behavior: $z \mapsto -z$.
Symmetry element name / interpretation: Inversion (center of symmetry at origin) — maps $(x, y, z)$to $(-x, -y, -z)$.

Together these generate the 6_3 screw axis and the mirror/inversion element that defines P6_3/m.

10)

```
loop_
    _atom_site_aniso_label
    _atom_site_aniso_U_11
    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_12
    _atom_site_aniso_U_13
    _atom_site_aniso_U_23
    CaI 0.01046 0.01046 0.00503 0.00523 0.00000 0.00000
    CaII 0.00709 0.00709 0.00743 0.00337 0.00000 0.00000
    P 0.00607 0.00574 0.00647 0.00337 0.00000 0.00000
    OI 0.01249 0.00979 0.01319 0.00844 0.00000 0.00000
    OII 0.00607 0.00945 0.02325 0.00337 0.00000 0.00000
```

OIII 0.03003 0.01451 0.01271 0.01485 -0.01081 -0.00739
O-h 0.00877 0.00877 0.02277 0.00439 0.00000 0.00000
H 0.04353 0.04353 0.02493 0.02177 0.00000 0.00000

- ***loop_:*** begins anisotropic displacement parameter (ADP) table for atoms that have anisotropic thermal parameters reported.
- ***_atom_site_aniso_label:*** label matching an atom label in the coordinate list (e.g., CaI, P, OIII, O-h, etc.).
- ***_atom_site_aniso_U_11 ... _atom_site_aniso_U_33*** and ***_atom_site_aniso_U_12 ... _atom_site_aniso_U_23*** are components of the symmetric 3×3 anisotropic displacement tensor U (commonly given in Å² units). The matrix format is:

  [U11 U12 U13]
  [U12 U22 U23]
  [U13 U23 U33]
- Values specify the mean-square displacements of atoms along and between axes. Larger numbers indicate larger thermal motion or static disorder.

Example: OIII has non-zero off-diagonal U13 and U23 (negative values allowed), indicating correlated displacements or directional anisotropy.

Notes:

- Not all CIFs report anisotropic U; if absent, isotropic Uiso or Biso might be present instead
- Here, both O-h (hydroxyl oxygen) and H have anisotropic parameters (H unusually reported anisotropically; some databases do that for refined H positions).

11)

*loop_*
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y

_atom_site_fract_z
_atom_site_occupancy
_atom_site_type_symbol
_atom_site_attached_hydrogens
CaI 0.33333 0.66667 0.00140 1.00000 Ca 0
CaII 0.24650 0.99330 0.25000 1.00000 Ca 0
P 0.39850 0.36840 0.25000 1.00000 P 0
OI 0.32820 0.48460 0.25000 1.00000 O 0
OII 0.58710 0.46490 0.25000 1.00000 O 0
OIII 0.34340 0.25790 0.07040 1.00000 O 0
O-h 0.00000 0.00000 0.19600 0.50000 O 0
H 0.00000 0.00000 0.06080 0.50000 H 0

- loop_ starts the atom-site table.
- _atom_site_label: human-readable atom label used elsewhere (must match anisotropic labels if anisotropic data is given).
- _atom_site_fract_x, _atom_site_fract_y, _atom_site_fract_z: fractional coordinates within the unit cell (values typically between 0 and 1). Coordinates are given relative to the lattice vectors a, b, c.
- _atom_site_occupancy: occupancy (1.0 = full occupancy). Values <1 indicate partial occupancy or disorder. Here O-h and H have occupancy 0.5 (0.50000), indicating half-occupied positions (common for the hydroxyl channel in hydroxyapatite because of disorder or two alternative orientations).
- _atom_site_type_symbol: element symbol (Ca, P, O, H).
- _atom_site_attached_hydrogens: optional free-format integer (here 0 for all). Some CIFs include attached_hydrogens for organic molecules to indicate how many H are bonded; for inorganic the field is 0.

Interpretation of specific entries:

- CaI 0.33333 0.66667 0.00140 1.00000 Ca 0: Ca atom at (1/3, 2/3, 0.00140) with full occupancy. Fractional coordinates often

reflect symmetry special positions (1/3/2/3 typical for hexagonal).

- CaII 0.24650 0.99330 0.25000 1.00000 Ca 0: second calcium site.
- P 0.39850 0.36840 0.25000 1.00000 P 0: phosphorus position associated with phosphate tetrahedron.
- O-h and H both at (0,0, z) but with occupancy 0.5: represent hydroxyl O and H occupying the same channel but only half occupied per site (typical structural motif in hydroxyapatite where OH may be disordered).